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Influence of self-affine and mound roughness on the surface impedance and skin depth of conductive materials

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Abstract

In this work, we explore the influence of self-affine and mound surface roughness on the surface impedance and skin depth. For self-affine roughness, the surface impedance and skin depth increases with decreasing the roughness exponent H (for $k_F\xi \gg 1$ with k_F the Fermi wave-vector), and/or increasing roughness ratio w/ξ , where w is the rms roughness amplitude and ξ the in-plane roughness correlation length. For mound roughness, the surface impedance and skin depth decrease monotonically with increasing average mound separation λ when $\lambda > \zeta$ with ζ the correlation length (assuming $k_F\zeta \gg 1$), while for $\lambda < \zeta$ they are both decreased with increasing λ .

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1. Introduction

The presence of material defects and deviations of surfaces/interfaces from flatness can alter drastically device operation [1,2]. Moreover, many new proposed device geometries require the growth of films with high quality, where kinetic effects can induce surface roughness depending on the material, the substrate, and the growth conditions. The latter creates an impetus for proper roughness quantification in the description of electrical processes that occur in the vicinity of non-flat surfaces/interfaces. Indeed, roughness effects on electrical properties appear in a diverse variety of cases [3–9]. For example, random rough surfaces have been shown to influence drastically the image potential of a charge situated in the vicinity of the interface plane between vacuum and a dielectric [3], as well as inversion layers at semiconductor/oxide interfaces, because roughness induces a shift of the electronic levels [4]. Also surface/interface roughness has been shown to influence strongly the electrical conductivity of semiconducting

and metallic thin film [5], as well as the electric field breakdown mechanism at a metal/insulator interface [6].

Furthermore, surface roughness influences the skin depth and cyclotron resonance phenomena in metals [7–9]. Alternatively, these phenomena could serve as experimental probes of physical processes on metal surfaces [7]. An electron loses any memory from the surface at distances greater than the bulk mean free path λ_p . Nevertheless, the mean free path λ_p can be larger than the skin depth or the sample dimensions at low temperatures, and for nearly perfect crystals. Thus, the electron will remember the surface in the region where it interacts with the electric field even relatively far from the surface boundary [7].

So far morphology effects on the skin effect and surface impedance have been considered only in terms of a Gaussian height–height correlation $C(r) = w^2 \times \exp(-r^2/\xi^2)$ with $r = (x, y)$ the in-plane position vector, w the rms roughness amplitude, and ξ the in-plane roughness correlation length [7]. However, a wide variety of morphology studies in thin films reveals the existence of a more complicated morphology, which is characterised in many cases by a roughness exponent $0 < H < 1$ at short length scales ($r < \xi$) [10,11], which describes the degree of surface irregularity. Although the self-affine

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morphology results during film growth due to noise induced roughening, the existence of an asymmetric step-edge diffusion barrier (Schwoebel barrier) [12,13], which inhibits the downhill diffusion of incoming atoms, can lead to the creation of mounds. The mound morphology appears in the form of multilayer stepped-structure, and it is characterised by a roughness exponent $H = 1$ [12,13].

Therefore, in this work we will explore roughness effects on the surface impedance and skin depth for self-affine and mound surface roughness, because of their wide applicability in describing rough morphologies in real thin film systems. Our calculations will be based on phenomenological roughness models, which, however, can capture the essence of the complexity for the rough surfaces under consideration.

2. Surface impedance and skin effect theory

When a conductor is placed in an external electromagnetic field, a skin layer is formed in the vicinity of the conductor surface with dimensions, depending on the penetration depth of the field. Here, it is assumed an electric field $E_z = E(z)\exp(-j\omega t)$ that acts on a rough metal surface (occupying the half-space $z > 0$) along the z -direction, which is normal to the surface. In the absence of a magnetic field and linear dependence on the electric field E_z , the solution of the Boltzmann Eq. [7] $v_c(\partial f/\partial z) + (\tau^{-1} - j\omega)f = -ev_c E_c(z)(df_0/d\varepsilon)$ yields the non-equilibrium electron distribution function f ($c = x, y$), with f_0 the Fermi–Dirac distribution function, ε the electron energy, v_c the electron velocity, and τ the bulk relaxation function.

If the electric field frequency is such that $\omega \ll \omega_0$ with ω_0 the plasma frequency and neglecting the displacement current, the Maxwell's equations yield $d^2 E_c/dz^2 = -4\pi j\omega(j_c(z)/c_1^2)$ where the electric current j_c is given by $j_c = (e/4\pi^3) \int (v_c f / |v_z|) d^2 p d\varepsilon$ with p the electron momentum, and c_1 the velocity of light [7]. The quantity that is measured experimentally is the surface impedance, which is defined by the relation [7]

$$Z = E_c(z=0)/\int j_c(z)dz, \quad (1)$$

and depends on the type of the skin effect (normal or anomalous). The calculations in the following apply for degenerate electron gas or $df_0/d\varepsilon = -\delta(\varepsilon - \varepsilon_F)$ with ε_F the Fermi energy.

2.1. Normal skin effect

This is the case for large skin depths or $|\delta| \gg |\lambda_{pf}|$, where $\lambda_{pf} = v_F(\tau^{-1} - j\omega)^{-1}$ ($v_F = p_F/m$ is the Fermi velocity). For $\omega\tau \ll 1$ we have $\lambda_{pf} \approx \lambda_p$, while in the opposite case $2\pi\lambda_{pf}$ is the path the electrons move within a field period. To first order in perturbation theory the surface impedance Z is

given by [7]

$$Z = \frac{4\pi\omega\delta}{ic_1^2} \left(1 + \frac{\lambda_{pf}}{\delta} k \right), \quad (2a)$$

$$k = \begin{cases} \frac{1}{10} Q; & Q = \frac{k_F}{\pi^2} \langle |h(0)|^2 \rangle \int \sqrt{k_F^2 - p_s^2} d^2 p_s, \text{ if } \xi k_F \ll 1 \\ \frac{3}{16} Q_1; & Q_1 = \frac{1}{\pi^2} \int_{0 < p_s < k_F} p_s^2 \langle |h(p_s)|^2 \rangle d^2 p_s, \text{ if } \xi k_F \gg 1 \end{cases} \quad (2b)$$

with $\delta = (c/\omega_0)(iv_F/\omega\lambda_{pf})^{1/2}$ the skin depth for a flat surface, and ξ a lateral roughness correlation length, which will be specified better in the following paragraphs. p_s is the in-plane electron wave-vector, and $\langle |h(\vec{p}_s)|^2 \rangle$ is the surface roughness spectrum assuming $h(\vec{p}_s)$ to be the Fourier transform of the real surface height $h(\vec{r})$. In deriving Eq. (2) it has been assumed isotropic roughness in the xy -plane. The skin depth δ for a flat surface in Eq. (2) is calculated from the principal value of the square root since λ is a complex [7]. Furthermore, if we rewrite the impedance as $Z = 4\pi\omega\delta_{eff}/ic_1^2$, we define an effective skin depth δ_{eff} that incorporates the presence of roughness so that

$$\delta_{eff} = \delta \left(1 + \frac{\lambda_{pf}}{\delta} k \right). \quad (3)$$

2.2. Anomalous skin effect

This is the case for small skin depths or $|\delta| \ll |\lambda_{pf}|$. The surface impedance is given by [7]

$$Z = 8\pi(1 + j\sqrt{3}) \frac{\omega\delta}{3^{3/2}c_1^2} + \frac{4\pi\omega\delta}{c_1^2} \tilde{k}, \quad (4a)$$

$$\tilde{k} = \begin{cases} (\sqrt{3} - j)Qg_1\delta/c_1^2\lambda_{pf}, & \text{if } k_F\xi \ll 1 \\ (1 - j\sqrt{3})Q_1g_2\lambda_{pf}^2/\delta^2c_1^2, & \text{if } k_F\xi \gg 1, \end{cases} \quad (4b)$$

with $\delta = (4p_Fc_1^2/3\pi m\omega\omega_0^2)^{1/3}$, $g_1 = 4/27$ and $g_2 = 8.7 \times 10^{-3}$. We define an effective skin depth δ_{eff} so that $Z = 8\pi(1 + j\sqrt{3})\omega\delta_{eff}/3^{3/2}c_1^2$ with

$$\delta_{eff} = \delta \begin{cases} [1 + (\delta/\lambda_{pf})\hat{k}], & \text{if } k_F\xi \ll 1, \\ [1 + (\lambda_{pf}^2/\delta^2)\hat{k}], & \text{if } k_F\xi \gg 1, \end{cases} \quad (5)$$

$$\hat{k} = \frac{3^{3/2}}{2(1 + j\sqrt{3})} \begin{cases} (\sqrt{3} - j)Qg_1, & \text{if } k_F\xi \ll 1, \\ (1 - j\sqrt{3})Q_1g_2, & \text{if } k_F\xi \gg 1. \end{cases}$$

3. Results–discussion

In Eqs. (2)–(5) the knowledge of the factors Q and Q_1 is required to evaluate surface roughness effects on the surface impedance Z and the effective skin depth δ_{eff} .

This is achieved by proper knowledge of the surface roughness spectra.

3.1. Self-affine rough surfaces

A wide variety of rough surfaces/interfaces are well described by a kind of roughness associated with self-affine fractal scaling [9]. Physical processes that produce such surfaces/interfaces include vapour/chemical deposition, molecular-beam-epitaxy, erosion, etc. [10]. In this case, $\langle |h(p)|^2 \rangle$ scales as [10] $\langle |h(p)|^2 \rangle \propto p^{-2-2H}$ if $p\xi \gg 1$, and $\langle |h(p)|^2 \rangle \propto \text{const}$ if $p\xi \ll 1$. Smaller values of $0 < H < 1$ characterise more jagged or irregular surfaces at short roughness wavelengths ($< \xi$). This scaling behaviour can be described by the simple model [14]

$$\langle |h(p)|^2 \rangle = \frac{1}{2\pi} \frac{w^2 \xi^2}{(1 + ap^2 \xi^2)^{1+H}} \quad (6)$$

with $a = (1/2H)[1 - (1 + aQ_c^2 \xi^2)^{-H}]$ if $0 < H < 1$, and $a = (1/2)\ln[1 + aQ_c^2 \xi^2]$ if $H = 0$. $Q_c = \pi/a_0$ with a_0 the atomic spacing. Other roughness models, which satisfy the self-affine scaling relations, can be found in Refs. [11,15]. For self-affine roughness we have upon substitution of Eq. (6) into Eq. (2b) the analytic forms

$$Q^{\text{SF}} = w^2 \xi^2 k_F^4 / 3\pi^2, \quad \text{if } k_F \xi \ll 1, \quad (7a)$$

$$Q_1^{\text{SF}} = \frac{w^2}{2\pi^2 a^2 \xi^2} \left\{ \frac{1}{1-H} [(1 + ak_F^2 \xi^2)^{1-H} - 1] + \frac{1}{H} [(1 + ak_F^2 \xi^2)^{-H} - 1] \right\}, \quad \text{if } k_F \xi \gg 1. \quad (7b)$$

For the limiting cases $H = 0$ and 1 one has to employ the identity $\ln(X) = \lim_{c \rightarrow 0} (1/c)(X^c - 1)$ to obtain the proper asymptotic limits. Indeed, we obtain

$$Q_1^{\text{SF}(H=0)} = \frac{w^2}{2\pi^2 a^2 \xi^2} \{ ak_F^2 \xi^2 + \ln(1 + ak_F^2 \xi^2) \}, \quad (7c)$$

and

$$Q_1^{\text{SF}(H=1)} = \frac{w^2}{2\pi^2 a^2 \xi^2} \{ \ln(1 + ak_F^2 \xi^2) + [(1 + ak_F^2 \xi^2)^{-1} - 1] \}. \quad (7d)$$

3.2. Mound rough surfaces

Mound surfaces have been described in the past by the rms roughness amplitude w , the system correlation length ξ which determines how randomly the mounds are distributed on the surface, and the average mound separation λ [13]. In terms of this model $\langle |h(p)|^2 \rangle$ is given by [13]

$$\langle |h(p)|^2 \rangle = \frac{w^2 \xi^2}{4\pi} e^{-(4\pi^2 + p^2 \lambda^2)(\xi^2/4\lambda^2)} I_0(\pi p \xi^2/\lambda) \quad (8)$$

with $I_0(x)$ the zero order modified Bessel function of first kind. The correlation function $C(r) = \langle h(r)h(0) \rangle$ ($\propto \int \langle |h(p)|^2 \rangle e^{-ipr} d^2p$) associated to Eq. (8) has an oscillatory behaviour for $\xi \geq \lambda$ (significant Schwoebel barrier effect during roughness growth) leading to a characteristic satellite ring at $q = 2\pi/\lambda$ for $\langle |h(p)|^2 \rangle$ [13]. For mound roughness we obtain for Q upon substitution of Eq. (8) a simple analytic form, while for Q_1 we obtain an analytic form only upon extension of the integration from 0 to $+\infty$ (for $k_F \xi \gg 1$). Thus, we obtain

$$Q^{\text{M}} = k_F^4 w^2 \xi^2 e^{-\pi^2 \xi^2/\lambda^2} / 6\pi^2, \quad (9a)$$

$$Q_1^{\text{M}} = \frac{4w^2}{\pi^2 \xi^2} \left(1 + \frac{\pi^2 \xi^2}{\lambda^2} \right). \quad (9b)$$

3.3. Calculations for self-affine and mound roughness

The calculations were performed for roughness amplitude $w = 0.5$ nm, and Fermi wave-vector $k_F = 5 \text{ nm}^{-1}$ so that $k_F \xi \gg 1$ and $k_F \lambda \gg 1$ for any physical lateral length scales $\xi, \lambda \gg a_0$ with a_0 in the order of the atomic spacing. In Fig. 1 we show the dependence of the factor k on the roughness ratio w/ξ for various values of the roughness exponent H . Indeed, with decreasing roughness exponent H ($0 < H < 1$), the magnitude of the factor k increases monotonically more than an order of magnitude as is also shown in Fig. 2. The latter reflects the fact that as the surface becomes rougher at short wavelengths (smaller H), the electron scattering becomes stronger corresponding to higher values of the factor k (or equivalently Q_1). Similar behaviour takes place with increasing long wavelength roughness ratio w/ξ . Nevertheless, for small roughness exponents H the effect of the ratio w/ξ is significantly less pronounced indicating dominance of short wave length roughness in the scattering process. Therefore, as Figs. 1 and 2 indicate, for small roughness exponents H (< 0.5) and large roughness ratios w/ξ (~ 0.1), the surface roughness has

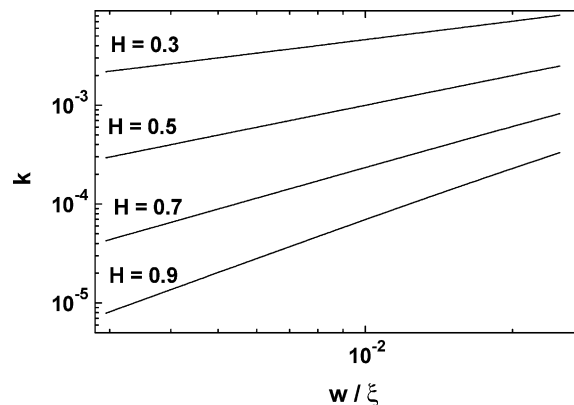


Fig. 1. Factor k vs. the long wavelength roughness ratio w/ξ ($k_F \xi \gg 1$) for various roughness exponents H .

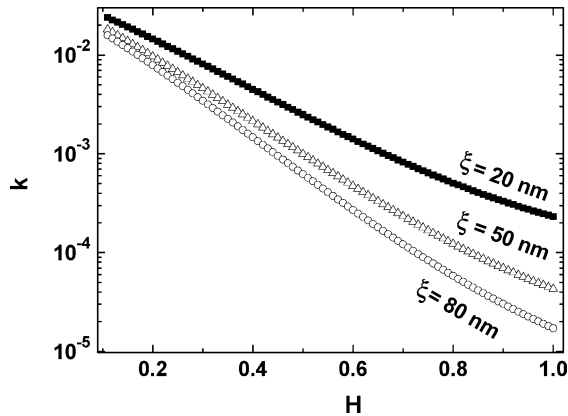


Fig. 2. Factor k vs. roughness exponent H for various correlation lengths ξ ($k_F \xi \gg 1$).

significant contribution on the impedance Z and the effective skin depth δ_{eff} simply through the factor k .

Since, in the normal skin effect the roughness contribution on the surface impedance Z and skin depth δ_{eff} is proportional to $\sim (|\lambda_{\text{pf}}|/|\delta|)k$ for $k_F \xi \gg 1$, the roughness effect will be diminished since $|\delta| \gg |\lambda_{\text{pf}}|$. On the other hand, in the anomalous skin effect or $|\delta| \ll |\lambda_{\text{pf}}|$, we obtain a surface impedance Z and a skin depth δ_{eff} that depends on the roughness as $\sim (|\lambda_{\text{pf}}|^2/|\delta|^2)|\tilde{k}|$ for $k_F \xi \gg 1$. Therefore, since $|\delta| \ll |\lambda_{\text{pf}}|$ the surface roughness will have significant effect on the impedance Z and skin depth δ_{eff} for small roughness exponents ($H < 0.5$) and/or significantly large ratios w/ξ (~ 0.1) in the anomalous skin effect case ($|\delta| \ll |\lambda_{\text{pf}}|$).

For mound roughness, Fig. 3 shows the behaviour of the factor k as a function of the ratio w/ξ for various mound separations λ . For large values of the average mound separation λ the factor k (or equivalently Q_1) increases monotonically with increasing ratio w/ξ (or decreasing system correlation length ξ for w fixed). Thus, for $\xi < \lambda$, where the Schwoebel barrier is insignificant during roughness growth, the behaviour of the factor k is similar to that of self-affine roughness (corresponding to the case of large

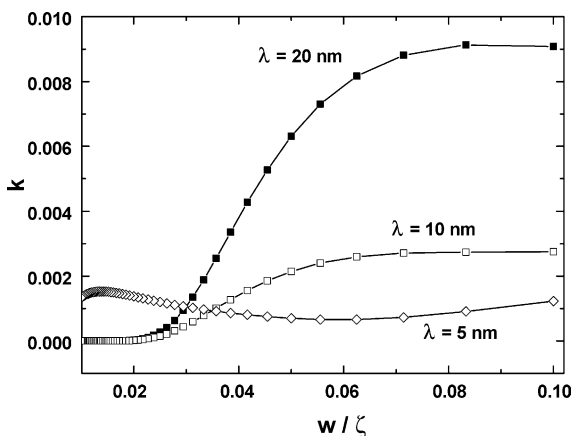


Fig. 3. Factor k vs. the long wavelength roughness ratio w/ξ ($k_F \xi \gg 1$) for various average mound separations λ .

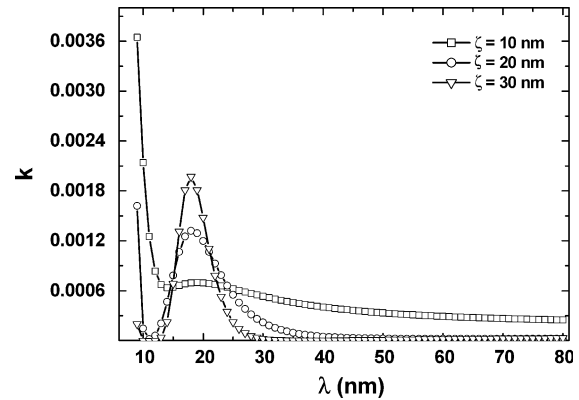


Fig. 4. Factor k vs. the average mound separation λ for various correlation lengths ξ ($k_F \xi \gg 1$).

roughness exponents $H \sim 1$). However, for smaller average mound separations λ , where the Schwoebel barrier is more dominant during growth, the factor k varies less in magnitude with increasing roughness ratio w/ξ . The value of the factor k in Fig. 3 for $\lambda = 5$ nm is higher than that of the other curves for low ratios w/ξ ($\ll 1$) since in this case we also have $\lambda \ll \xi$ (strong Schwoebel regime during roughness growth where oscillations of the roughness height–height correlation function take place at lateral length scales $> \xi$). Therefore, for mound surfaces with $\xi > \lambda$, the roughness effects have certainly a more complex contribution on the surface impedance Z and skin depth δ_{eff} from that of self-affine rough surfaces.

In order to gain further insight on the influence of mound roughness we plot in Fig. 4 the factor k vs. the average mound separation λ for various values of the system correlation length ξ . Indeed, for small ξ such that $\lambda > \xi$, the factor k decreases smoothly with increasing λ or decreasing ratio w/λ (for fixed w) indicating surface smoothing, and therefore less charge scattering by roughness. However, with increasing system correlation length ξ , the factor k shows an oscillatory behaviour, which is prominent for $\lambda < \xi$ accompanied by a gradual decrement. The oscillations increase in amplitude with increasing ξ . The latter manifests the presence of a stronger Schwoebel barrier effect during roughness growth that lead to an oscillatory behaviour for the corresponding height–height correlation function at large length scales (or $r > \xi$) [13]. This morphological oscillation is expected to influence electron scattering as Fig. 4 indicates.

4. Conclusions

In summary, we explored the influence of surface roughness on the surface impedance and skin depth for self-affine and mound roughness. For self-affine rough surfaces, the effective skin depth δ_{eff} and surface impedance Z increase monotonically with decreasing roughness exponent H and/or increasing long wavelength roughness

ratio w/ξ . Indeed, for relatively large correlation lengths $\xi(k_F\xi \gg 1)$, the roughness details at short wave lengths (effect of the roughness exponent H) become rather dominant. For mound rough surfaces, the skin depth and surface impedance show more complex dependence as a function of the system correlation length $\xi(k_F\xi \gg 1)$ and the average mound separation λ depending on the magnitude of the ratio ξ/λ . At any rate, the roughness contributions on the effective skin depth δ_{eff} and surface impedance Z will show distinct characteristics associated with the formation of a specific rough growth front when the characteristics lateral length scales are larger than $1/k_F$.

Finally, we should point out that it would be interesting to apply the present theoretical results to studies of surface impedance measurements on self-affine and mound rough surfaces. Examples of self-affine roughness include the room temperature growth of Ag [16], Au [17], Pt [18] onto quartz (or Si-oxide), etc. For a review on various systems see more detailed results in Refs. [10,17]. On the other hand, for mound rough surfaces examples include the growth of Ag/Ag(111), the growth of Cu/Cu(100), the growth of Fe/Fe(001), the growth of Pt/Pt(111) [19], etc. Moreover, variation of deposition parameters (deposition rate, substrate temperature, film thickness) can alter the solid thin film (substrate) roughness parameters [10], which in turn can be used as an additional manner to influence and modulate surface impedance related phenomena.

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